Implications of Coverage-Dependent O Adsorption for Catalytic NO Oxidation on the Late Transition Metals

Supplemental Information

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A unique identifier for each formation energy calculation, fractional coverage, supercell vectors, adsorbate arrangement, and k-point mesh size are given in table A.1.

Table A.1. Summary of supercell arrangements and adsorbate configurations used in formation energy calculations.

ID#	Coverage N_{ads}/N_{site}	Supercell Vectors	Adsorbate Vectors	k-Point	E_{frm} (eV/site)										
					Ru	Os	Co	Rh	Ir	Ni	Pd	Pt	Cu	Ag	Au
110	0/1	a,b,c		12,12, 1	1.001	1.178	0.750	0.806	0.914	0.651	0.567	0.631	0.464	0.351	0.343
111	1/1	a,b,c		12,12, 1	-1.199	-0.949	-1.068	-0.513	-0.140	-0.322	0.305	0.393	0.589	1.308	1.364
112	0/2	a,a+2b,c		10, 6, 1	1.015	1.178	0.743	0.809	0.915	0.647	0.558	0.632	0.462	0.349	0.341
113	1/2	a,a+2b,c		10, 6, 1	-0.340	-0.147	-0.558	-0.135	0.075	-0.409	0.026	0.134	-0.062	0.354	0.455
114	2/2	a,a+2b,c		10, 6, 1	-1.199	-0.960	-1.071	-0.514	-0.144	-0.324	0.299	0.392	0.597	1.316	1.363
115	0/3	3a+2b,-3a-b,c		10,10, 1	1.011	1.173	0.743	0.793	0.904	0.656	0.553	0.640	0.464	0.350	0.344
116	1/3	3a+2b,-3a-b,c		10,10, 1	0.102	0.272	-0.132	0.154	0.341	-0.063	0.183	0.302	0.099	0.346	0.358
117	2/3	3a+2b,-3a-b,c		10,10, 1	-0.651	-0.474	-0.840	-0.317	-0.070	-0.517	0.059	0.170	.	0.613	0.667
118	3/3	3a+2b,-3a-b,c		10,10, 1	-1.196	-0.964	-1.070	-0.528	-0.149	-0.303	0.298	0.397	0.604	1.330	1.370
119	0/3	a-b,a+2b,c		7, 7, 1	1.014	1.158	0.745	0.804	0.920	0.658	0.573	0.653	0.461	0.346	0.337
120	1/3	a-b,a+2b,c		7, 7, 1	0.109	0.288	-0.226	0.132	0.318	-0.190	0.143	0.262	-0.069	0.213	0.344
121	2/3	a-b,a+2b,c		7, 7, 1	-0.653	-0.502	-0.779	-0.258	-0.081	-0.526	0.023	0.102	0.040	0.579	0.613
122	3/3	a-b,a+2b,c		7, 7, 1	-1.187	-0.974	-1.072	-0.510	-0.135	-0.318	0.308	0.395	0.600	1.324	1.358
124	0/4	2a,a+2b,c		5, 6, 1	1.014	1.195	0.742	0.804	0.913	0.651	0.565	0.638	0.463	0.350	0.340
125	1/4	2a,a+2b,c		5, 6, 1	0.281	0.467	-0.006	0.279	0.444	-0.002	0.225	0.323	0.038	0.220	0.314
126	2/4	2a,a+2b,c	a-b	5, 6, 1	-0.302	-0.114	-0.571	-0.089	0.103	-0.425	0.046	0.149	-0.078	0.365	0.480
127	3/4	2a,a+2b,c		5, 6, 1	-0.817	-0.627	-0.892	-0.359	-0.117	-0.518	0.054	0.158	0.162	0.754	0.812
128	4/4	2a,a+2b,c		5, 6, 1	-1.198	-0.954	-1.068	-0.517	-0.145	-0.323	0.299	0.396	0.602	1.325	1.360
129	0/4	2a,2b,c		6, 6, 1	1.002	1.185	0.754	0.803	0.916	0.655	0.574	0.633	0.472	0.366	0.351
130	1/4	2a,2b,c		6, 6, 1	0.237	0.434	-0.009	0.266	0.445	-0.005	0.223	0.309	0.026	0.222	0.316
131	2/4	2a,2b,c	a	6, 6, 1	-0.347	-0.150	-0.551	-0.142	0.072	-0.406	0.034	0.133	-0.067	0.357	0.458
132	3/4	2a,2b,c		6, 6, 1	-0.839	-0.628	-0.895	-0.392	-0.126	-0.512	0.052	0.170	0.191	0.788	0.876
133	4/4	2a,2b,c		6, 6, 1	-1.207	-0.947	-1.065	-0.517	-0.148	-0.320	0.307	0.397	0.607	1.330	1.357
134	0/4	a,2a+4b,c		10, 3, 1	1.014	1.183	0.741	0.803	0.912	0.652	0.566	0.635	0.463	0.345	0.340
135	1/4	a,2a+4b,c		10, 3, 1	0.330	0.501	0.080	0.324	0.480	0.110	0.286	0.364	0.183	0.335	0.344
136	2/4	a,2a+4b,c	a+b	10, 3, 1	-0.239	-0.076	-0.460	-0.041	0.159	-0.257	0.157	0.237	.	.	.
137	3/4	a,2a+4b,c		10, 3, 1	-0.797	-0.608	-0.943	-0.380	-0.113	-0.514	0.101	0.188	.	.	.
138	4/4	a,2a+4b,c		10, 3, 1	-1.200	-0.954	-1.067	-0.516	-0.145	-0.323	0.299	0.393	0.600	1.320	1.351
139	0/5	-2a-3b,3a+2b,c		6, 6, 1	1.005	1.179	0.745	0.803	0.923	0.658	0.568	0.643	0.465	0.351	0.339
140	1/5	-2a-3b,3a+2b,c		6, 6, 1	0.409	0.591	0.143	0.380	0.550	0.131	0.290	0.390	0.124	0.249	0.315
141	2/5	-2a-3b,3a+2b,c	a+2b	6, 6, 1	-0.084	0.107	-0.386	0.026	0.227	-0.308	0.086	0.200	-0.112	0.247	0.370
142	2/5	-2a-3b,3a+2b,c	b	6, 6, 1	-0.083	0.082	-0.330	0.061	0.256	-0.224	0.140	0.235	-0.007	0.333	0.407
143	3/5	-2a-3b,3a+2b,c	b,-a	6, 6, 1	-0.523	-0.340	-0.744	-0.214	0.014	-0.496	0.053	0.160	.	0.536	0.616
144	3/5	-2a-3b,3a+2b,c	a+2b,b	6, 6, 1	-0.532	-0.364	-0.688	-0.205	0.000	-0.478	0.028	0.116	0.009	0.500	0.539
145	4/5	-2a-3b,3a+2b,c		6, 6, 1	-0.902	-0.719	-0.941	-0.395	-0.128	-0.500	0.095	0.188	0.227	.	0.930
146	5/5	-2a-3b,3a+2b,c		6, 6, 1	-1.201	-0.963	-1.067	-0.511	-0.136	-0.321	0.302	0.395	0.605	1.333	1.357
147	0/5	-3a+2b,2a-3b,c		10,10, 1	1.014	1.176	0.743	0.797	0.919	0.659	0.568	0.638	0.460	0.345	0.337
148	2/5	-3a+2b,2a-3b,c	3a-3b	10,10, 1	0.008	0.163	-0.226	0.118	0.310	-0.079	0.232	0.291	.	0.454	0.466
149	2/5	-3a+2b,2a-3b,c	-a+b	10,10, 1	-0.081	0.102	-0.302	0.043	0.241	-0.203	0.127	0.228	0.024	0.340	0.384
150	3/5	-3a+2b,2a-3b,c	-a+b,3a-3b	10,10, 1	-0.527	-0.345	-0.728	-0.240	-0.003	-0.473	0.051	0.143	.	0.496	0.559
151	3/5	-3a+2b,2a-3b,c	-a+b,2a-2b	10,10, 1	-0.441	-0.277	-0.619	-0.161	0.073	-0.315	0.161	0.227	.	.	.
152	5/5	-3a+2b,2a-3b,c		10,10, 1	-1.197	-0.964	-1.069	-0.514	-0.139	-0.320	0.301	0.391	0.606	1.329	1.353
153	0/6	-3a-b,-2b,c		4, 5, 1	1.011	1.190	0.744	0.797	0.898	0.659	0.556	0.640	0.457	0.352	0.333
154	2/6	-3a-b,-2b,c	-a+b	4, 5, 1	0.052	0.245	-0.218	0.120	0.307	-0.166	0.139	0.256	-0.033	0.249	0.354
155	3/6	-3a-b,-2b,c	-a-b,-2a-b	4, 5, 1	-0.322	-0.128	-0.566	-0.118	0.085	-0.418	0.033	0.152	-0.065	0.375	0.460
156	5/6	-3a-b,-2b,c		4, 5, 1	-0.961	-0.759	-0.975	-0.442	-0.151	-0.475	0.117	0.232	.	.	.

Table A.1 (cont.). Summary of supercell arrangements and adsorbate configurations used in formation energy calculations.

ID#	Coverage N_{ads}/N_{site}	Supercell Vectors	Adsorbate Vectors	k-Point	E_{frm} (eV/site)										
					Ru	Os	Co	Rh	Ir	Ni	Pd	Pt	Cu	Ag	Au
157	6/6	-3a-b,-2b,c		4, 5, 1	-1.199	-0.955	-1.071	-0.530	-0.150	-0.316	0.298	0.400	0.608	1.336	1.358
158	0/6	-b,6a+3b,c		10, 2, 1	1.013	1.179	0.742	0.804	0.909	0.654	0.555	0.644	0.463	0.344	0.344
159	3/6	-b,6a+3b,c	2a+b,a+b	10, 2, 1	-0.201	-0.037	-0.405	-0.020	0.194	-0.165	0.208	0.270	.	.	.
160	6/6	-b,6a+3b,c		10, 2, 1	-1.200	-0.958	-1.069	-0.531	-0.154	-0.323	0.299	0.400	0.605	1.331	1.353
161	0/6	a-b,3a+3b,c		6, 3, 1	1.004	1.161	0.745	0.804	0.913	0.651	0.565	0.638	0.466	0.348	0.338
162	1/6	a-b,3a+3b,c		6, 3, 1	0.518	0.686	0.241	0.452	0.597	0.213	0.336	0.423	0.181	0.260	0.318
163	2/6	a-b,3a+3b,c	a+b	6, 3, 1	0.060	0.241	-0.216	0.135	0.313	-0.167	0.150	0.247	-0.038	0.237	0.341
164	3/6	a-b,3a+3b,c	a+b,-b	6, 3, 1	-0.309	-0.129	-0.558	-0.090	0.090	-0.413	0.054	0.148	-0.066	0.369	0.453
165	4/6	a-b,3a+3b,c	a+b,-b,a	6, 3, 1	-0.640	-0.457	-0.836	-0.279	-0.050	-0.515	0.069	0.166	.	.	0.693
166	5/6	a-b,3a+3b,c		6, 3, 1	-0.957	-0.759	-0.975	-0.418	-0.145	-0.478	0.125	0.221	.	.	0.999
167	6/6	a-b,3a+3b,c		6, 3, 1	-1.205	-0.956	-1.075	-0.516	-0.145	-0.321	0.300	0.397	0.605	1.326	1.359
168	0/7	-3a-b,a-2b,c		4, 4 ,1	1.030	1.191	0.747	0.798	0.914	0.656	0.581	0.636	0.471	0.350	0.342
169	4/7	-3a-b,a-2b,c	2a+b,a+b,b	4, 4, 1	-0.471	-0.275	-0.702	-0.195	0.032	-0.485	0.049	0.147	.	.	0.542
170	6/7	-3a-b,a-2b,c		4, 4, 1	-0.996	-0.785	-0.992	-0.444	-0.139	-0.464	0.149	0.236	0.318	.	.
171	7/7	-3a-b,a-2b,c		4, 4, 1	-1.195	-0.944	-1.069	-0.516	-0.132	-0.317	0.306	0.398	0.605	1.331	1.348
172	0/7	-a+3b,-a-4b,c		6, 6, 1	1.008	1.175	0.742	0.799	0.918	0.659	0.568	0.636	0.463	0.347	0.340
173	1/7	-a+3b,-a-4b,c		6, 6, 1	0.585	0.759	0.310	0.496	0.646	0.281	0.372	0.452	0.217	0.271	0.313
174	2/7	-a+3b,-a-4b,c	a-b	6, 6, 1	0.188	0.379	-0.104	0.213	0.393	-0.083	0.193	0.294	-0.009	0.218	0.325
175	3/7	-a+3b,-a-4b,c	a-2b,a-b	6, 6, 1	-0.169	0.028	-0.440	-0.028	0.174	-0.340	0.072	0.176	-0.107	0.273	0.383
176	4/7	-a+3b,-a-4b,c	a-2b,a-b,a	6, 6, 1	-0.480	-0.304	-0.650	-0.188	0.017	-0.453	0.031	0.118	-0.015	0.455	0.503
177	3/7	-a+3b,-a-4b,c	a-b,a+b	6, 6, 1	-0.141	0.046	-0.426	0.003	0.192	-0.327	0.088	0.185	-0.082	0.296	0.411
178	4/7	-a+3b,-a-4b,c	a-2b,a,a+b	6, 6, 1	-0.431	-0.267	-0.626	-0.153	0.069	-0.374	0.118	0.200	.	.	0.613
179	4/7	-a+3b,-a-4b,c	a-2b,a,-2b	6, 6, 1	-0.465	-0.289	-0.672	-0.168	0.019	-0.477	0.039	0.122	-0.033	0.458	0.530
180	5/7	-a+3b,-a-4b,c	a-2b,a-b,a,-2b	6, 6, 1	-0.756	-0.581	-0.847	-0.320	-0.103	-0.521	0.044	0.132	0.119	0.683	0.724
181	6/7	-a+3b,-a-4b,c		6, 6, 1	-0.995	-0.796	-0.985	-0.438	-0.147	-0.452	0.156	0.243	.	.	.
182	7/7	-a+3b,-a-4b,c		6, 6, 1	-1.202	-0.962	-1.062	-0.509	-0.134	-0.311	0.311	0.400	0.612	1.333	1.351
183	0/8	-3a+b,a-3b,c		5, 5, 1	1.013	1.185	0.746	0.801	0.912	0.652	0.572	0.631	0.471	0.361	0.347
184	2/8	-3a+b,a-3b,c	b	5, 5, 1	0.297	0.476	0.021	0.291	0.459	0.033	0.248	0.334	0.085	0.265	0.339
185	4/8	-3a+b,a-3b,c	3a-2b,2a-b,a-b	5, 5, 1	-0.326	-0.132	-0.561	-0.122	0.084	-0.416	0.038	0.138	-0.072	0.359	0.447
186	8/8	-3a+b,a-3b,c		5, 5, 1	-1.198	-0.962	-1.065	-0.517	-0.146	-0.319	0.305	0.397	0.605	1.327	1.353
187	0/8	-3a-2b,a-2b,c		4, 4, 1	1.013	1.199	0.746	0.792	0.902	0.657	0.573	0.642	0.463	0.352	0.342
188	4/8	-3a-2b,a-2b,c	2a+3b,a+3b,a+2b	4, 4, 1	-0.306	-0.110	-0.605	-0.115	0.091	-0.449	0.059	0.169	.	.	0.479
189	8/8	-3a-2b,a-2b,c		4, 4, 1	-1.200	-0.954	-1.066	-0.520	-0.141	-0.319	0.302	0.397	0.603	1.330	1.354
190	0/8	a-b,4a+4b,c		6, 3, 1	1.008	1.179	0.745	0.806	0.914	0.651	0.565	0.638	0.465	0.349	0.338
191	1/8	a-b,4a+4b,c		6, 3, 1	0.638	0.812	0.367	0.538	0.674	0.323	0.390	0.473	0.251	0.280	0.317
192	4/8	a-b,4a+4b,c	a+b,a+2b,2a+3b	6, 3, 1	-0.299	-0.120	-0.544	-0.085	0.101	-0.404	0.057	0.149	-0.070	0.361	0.458
193	5/8	a-b,4a+4b,c	a+b,a+2b,2a+3b,-a-b	6, 3, 1	-0.576	-0.409	-0.724	-0.226	-0.038	-0.499	0.024	0.107	0.016	0.517	0.552
194	7/8	a-b,4a+4b,c		6, 3, 1	-1.020	-0.816	-1.000	-0.450	-0.153	-0.444	0.165	0.260	.	.	.
195	8/8	a-b,4a+4b,c		6, 3, 1	-1.198	-0.953	-1.067	-0.517	-0.143	-0.320	0.300	0.397	0.604	1.328	1.358

Supercell geometries and coverages with more than one possible adsorbate arrangement indicate the relationships between initial and subsequent adsorbates (e.g., for configuration 143: the vector between the 1st and 2nd adsorbate is b; the vector between the 1st and 3rd adsorbate is -a). All k-point meshes are Γ-centered.

$a = (1,0,0) \quad b = \left(-\frac{1}{2}, \frac{\sqrt{3}}{2}, 0\right) \quad c = \left(0,0,\frac{20\sqrt{6}}{3}\right)$